6.0 Calculation of Risk or Allowable Waste Concentration

This section describes how IWAIR calculates risk or allowable waste concentration using the emission rate, dispersion factor, exposure factors, and health benchmarks described in previous sections.

6.1 Calculation of Risk or Hazard Quotient

IWAIR calculates risk for carcinogens and HQ for noncarcinogens. To calculate risk from a specified chemical to a specified receptor, IWAIR uses the following steps:

1. Calculate emission rates from user inputs or user-specified emission rates; the emission rates are chemical-specific and, if calculated by IWAIR, depend on user-specified waste concentrations.

2. Calculate dispersion factors from user inputs or user-specified dispersion factors; the dispersion factors are receptor-specific.

3. Calculate air concentrations from emission rates and dispersion factors; the air concentrations are chemical- and receptor-specific.

4. Calculate risks or HQs from air concentrations and, for carcinogens, exposure factors.

Calculation of emission rates and dispersion factors (Steps 1 and 2) is discussed in Sections 2 and 3 of this document. For Step 3, IWAIR calculates air concentration from WMU emission rates and dispersion factors, as follows:

$$C_{air,j} = (E_j \times 10^6) \times DF \qquad (6\text{-}1)$$

where

$C_{air,j}$ = air concentration of chemical j ($\mu g/m^3$)
E_j = volatile emission rate of chemical j (g/m^2-s)
10^6 = unit conversion ($\mu g/g$)
DF = dispersion factor ($[\mu g/m^3]/[\mu g/m^2$-s$]$).

For Step 4, IWAIR then uses this calculated air concentration, the exposure factors described in Section 4, and the health benchmarks described in Section 5 to calculate risk or HQ. The following subsections describe this calculation for carcinogens and noncarcinogens.

6.1.1   Calculation of Risk for Carcinogens

Risk for carcinogens is calculated as follows:

$$\text{Risk}_j = \frac{C_{air,j} \times 10^{-3} \times CSF_j \times EF}{AT \times 365} \times \sum_{i=1}^{5} \frac{IR_i \times ED_i}{BW_i} \tag{6-2}$$

where

10^{-3} = unit conversion (mg/μg)
Risk_j = individual risk for chemical j (unitless)
CSF_j = cancer slope factor for chemical j (per mg/kg-d)
i = index on age group (e.g., <1 yr, 1–5 yrs, 6–11 yrs, 12–19 yrs, Adult)
IR_i = inhalation rate for age group i (m^3/d)
ED_i = exposure duration for age group i (yr)
EF = exposure frequency (d/yr)
AT = averaging time (yr) = 70
365 = unit conversion (d/yr)
BW_i = body weight for age group i (kg).

Averaging time corresponds to a typical lifetime and is a fixed input to this equation because it must be consistent with the 70-year averaging time used to develop the CSF. This averaging time reflects the lifetime over which cancer risks are averaged. It is not related to the exposure duration (which is the length of time a receptor is exposed to a chemical) or the averaging period used for emission rates (which is the length of time over which emission rates are averaged; this is set to correspond to the exposure duration).

Equation 6-2 reflects calculation of carcinogenic risk for residents and must be modified slightly to calculate risk for workers. Exposure factors for adult workers are used in place of age-specific exposure factors for residents. Thus, the summation over age group, i, is not needed for workers.

IWAIR also calculates the cumulative risk for all carcinogens modeled in a run. This is a simple sum of the chemical-specific risks already calculated, as follows:

$$\text{CumRisk} = \sum_{j=1}^{n} \text{Risk}_j \tag{6-3}$$

where

CumRisk   =   cumulative individual risk for all carcinogens modeled (unitless)
j   =   index on chemical
n   =   number of carcinogens modeled.

6.1.2   Calculation of HQ for Noncarcinogens

The HQ for noncarcinogens, which is not dependent on exposure factors, is calculated as follows:

$$HQ_j = \frac{C_{air,j} \times 10^{-3}}{RfC_j} \qquad (6\text{-}4)$$

where

HQ_j =   hazard quotient for chemical *j* (unitless)
10^{-3} =   unit conversion (mg/µg)
RfC_j =   reference concentration for chemical *j* (mg/m^3).

No cumulative HQ is calculated for noncarcinogens. Such summing of HQs is appropriate only when the chemicals involved have the same target organ.

6.2   Calculation of Allowable Waste Concentration

The calculation of the allowable waste concentration from a target risk or HQ is somewhat more complex than the risk calculation for several reasons.

First, emission rates depend on whether the waste modeled is aqueous-phase or organic-phase. In risk calculation mode, the user establishes the waste type as an input, and IWAIR calculates emission rates and the ensuing risk or HQ for that waste type. In allowable concentration mode, IWAIR must determine whether to base the allowable concentration on an emission rate for an aqueous-phase waste or an organic-phase waste.

Second, if risk is linear with waste concentration, then emission rates may be calculated for a unit waste concentration, and air concentration and risk and HQ equations may be solved for waste concentration. This is the case for land application units, landfills, and waste piles. However, emission rates are not linear with waste concentration for aqueous-phase wastes in surface impoundments because of nonlinearities in biodegradation processes. In surface impoundments, biodegradation is first order at low concentrations and eventually becomes zero order at higher concentrations. The concentration at which this shift occurs is chemical-specific. This is not the case with organic-phase emissions from surface impoundments, because biodegradation is not modeled in that scenario because of model limitations. Therefore, for aqueous-phase wastes in surface impoundments, an iterative risk calculation approach must be used to calculate allowable waste concentration.

Finally, when solving the risk and HQ equations for waste concentration (or when iteratively solving the risk equations for increasing concentrations), care must be taken to ensure that the resulting concentration is within physical limits for the associated waste type.

The following subsections describe how allowable waste concentrations are calculated for land application units, landfills, and waste piles; how allowable waste concentrations are calculated for surface impoundments; and how IWAIR sets an allowable waste concentration that observes physical limitations.

6.2.1 Calculating Allowable Waste Concentrations for Land Application Units, Landfills, and Waste Piles

To calculate an allowable concentration, IWAIR uses the following steps:

1. Calculate unitized emission rates from user inputs or user-specified unitized emission rates; the emission rates are chemical-specific and correspond to a waste concentration of 1 mg/kg or mg/L; if calculated by IWAIR, unitized emission rates are also specific to waste type (i.e., aqueous- or organic-phase).

2. Calculate dispersion factors from user inputs or user-specified dispersion factors; the dispersion factors are receptor-specific.

3. Calculate target air concentrations from target risk or HQ, health benchmarks, and, for carcinogens, exposure factors; the air concentrations are chemical- and receptor-specific.

4. Calculate waste concentrations from air concentrations, dispersion factors, and unitized emission rates, for aqueous- and organic-phase wastes.

5. Choose an allowable concentration from the waste concentrations calculated for aqueous- and organic-phase wastes.

Calculation of emission rates and dispersion factors (Steps 1 and 2) is discussed in Sections 2 and 3 of this document. For Step 3, IWAIR uses the same underlying risk and HQ equations presented in Section 6.1 to calculate allowable concentration for land application units, landfills, and waste piles. Equations 6-2 (for risk) and 6-4 (for HQ) may be solved for air concentration. The risk or HQ in those equations becomes the target risk or HQ selected by the user.

For Step 4, IWAIR then uses an equation comparable to Equation 6-1 to relate air concentration to waste concentration. However, this equation must be adapted to reflect the use of a unitized emission rate associated with a waste concentration of 1 mg/kg. This new equation assumes that emissions are linear with waste concentration. The adapted equation is as follows:

$$C_{air} = (C_{waste} \times E_{unit} \times 10^6) \times DF \qquad (6\text{-}5)$$

where

C_{air} = air concentration ($\mu g/m^3$)
C_{waste} = waste concentration (mg/kg or mg/L)
E_{unit} = normalized volatile emission rate of constituent ([g/m^2-s]/[mg/kg] or [g/m^2-s]/[mg/L])
10^6 = unit conversion ($\mu g/g$)
DF = dispersion factor ([$\mu g/m^3$]/[$\mu g/m^2$-s]).

Equation 6-5 may be solved for waste concentration to calculate waste concentration from air concentration. This equation is then used with both an aqueous-phase emission rate and an organic-phase emission rate, to get an aqueous-phase waste concentration and an organic-phase waste concentration. Section 6.2.3 describes how IWAIR uses those two concentrations to set an allowable waste concentration (Step 5).

6.2.2   Calculating Allowable Waste Concentrations for Surface Impoundments

For organic-phase wastes in surface impoundments, emissions are linear with waste concentration, so waste concentration is calculated following Steps 1 to 4, as described in Section 6.2.1.

For aqueous-phase wastes in surface impoundments, emissions are not linear with waste concentration. Therefore, an iterative method adapted from the Newton-Raphson method was used in IWAIR.

The Newton-Raphson method is a commonly used formula for locating the root of an equation, i.e., the value of x at which f(x) is zero (Chapra and Canale, 1985). The method is based on the geometrical argument that the intersection of a tangent to a function at an initial guess, x_i, with the x-axis is a better approximation of the root than x_i. As illustrated in Figure 6-1, the method can be adapted to a nonzero target value of f(x), α; in this case, the intersection of the tangent with the line corresponding to $y = \alpha$ is used as the next approximation.

Mathematically, the slope of this tangent, f$'$(x_i) is given as follows:

$$f'(x_i) = \frac{f(x_i) - \alpha}{x_i - x_{i+1}}$$

(6-6)

where

$f'(x_i)$ = the slope of f(x) at x_i
$f(x_i)$ = the value of f(x) at x_i
α = the target value for f(x)
x_i = the initial guess for x
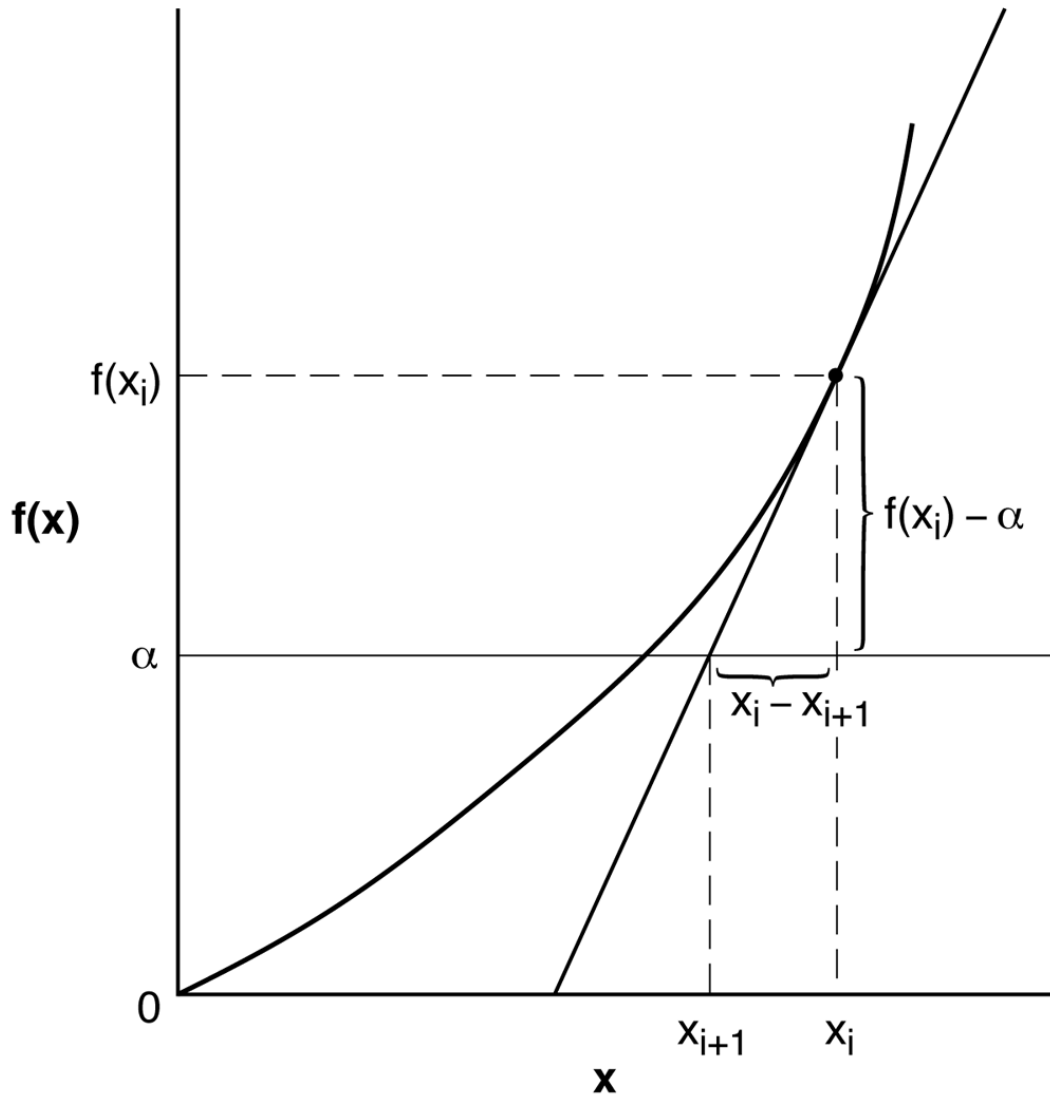x_{i+1} = the next approximation of x.

Figure 6-1. Graphical interpretation of the Newton-Raphson method.

This can be rearranged as follows to solve for x_{i+1}:

$$x_{i+1} = x_i - \frac{f(x_i) - \alpha}{f'(x_i)} \;.$$

(6-7)

Equation 6-7 gives an improved value of x for the next iteration; however, to use it, $f'(x_i)$ must first be estimated. This is done using finite difference methods:

$$f'(x_i) = \frac{f(x_i + \epsilon) - f(x_i)}{\epsilon}$$

(6-8)

where

$f(x_i + \epsilon)$ = the value of f(x) at $x_i + \epsilon$
ϵ = a small value relative to x_i.

For IWAIR, ϵ was set to $0.1x_i$.

This method can be applied iteratively until f(x) is within a predefined tolerance of the target, α. For IWAIR, the stopping criteria was set to f(x) = $\alpha \pm 1\%$.

For IWAIR, the variable x in the general Newton-Raphson method is waste concentration, and the function f(x) is the calculation of either risk or HQ based on waste concentration following the Steps 1 through 4 laid out in Section 6.1 for risk mode.

As for the other units, where risk is linear with waste concentration, both an aqueous-phase waste concentration (using the Newton-Raphsm method) and an organic-phase waste concentration (using the approach described in Section 6.2.1) are developed. Section 6.2.3 describes how IWAIR uses those concentrations to set an allowable waste concentration (Step 5).

6.2.3   Setting an Allowable Waste Concentration

The final step, Step 5, to setting an allowable waste concentration is to choose between the waste concentrations based on aqueous-phase emissions and organic-phase emissions and to ensure that the resulting concentration does not exceed physical limitations.

As discussed in Section 2, wastes are typically assumed to be aqueous phase (i.e., dilute wastes that partition primarily to water). However, aqueous-phase wastes are likely to occur in land application units, landfills, and waste piles only up to the soil saturation limit, and in surface impoundments up to the solubility of the chemical in water. At concentrations above the soil saturation or solubility limit, wastes are more likely to occur in organic phase, unless waste matrix effects allow supersaturated conditions to occur. Although it is possible for aqueous-phase wastes to exist with chemicals present above the saturation or solubility limit, this is an unusual occurrence. Therefore, IWAIR limits calculated allowable waste concentrations based on aqueous-phase emission rates to the soil saturation or solubility limit or lower. The solubility limit is a chemical-specific property and is included in the IWAIR chemical properties database. The soil saturation limit is dependent on site-specific factors, as well as chemical properties; therefore, IWAIR calculates it from user inputs as follows:

$$C_{sat} = \frac{S}{\rho_b} (K_d \times \rho_b + \epsilon_w + H' \times \epsilon_a) \tag{6-9}$$

where

C_{sat} = soil saturation limit (mg/kg)
S = solubility limit (mg/L)

ρ_b = bulk density of soil/waste matrix (kg/L)

K_d = soil-water partition coefficient (L/kg), calculated as shown below in Equation 6-10 for organic chemicals; this is an input for mercury

ϵ_w = water-filled soil porosity (unitless)

H' = dimensionless Henry's law constant (unitless = H/RT)

ϵ_a = air-filled soil porosity (unitless).

and

$$K_d = K_{oc} \times f_{oc} \qquad (6\text{-}10)$$

where

K_d = soil-water partition coefficient (L/kg)

K_{oc} = organic carbon partition coefficient (L/kg), calculated as shown below in Equation 6-11

f_{oc} = fraction organic carbon in waste (unitless).

Fraction organic carbon is set to a fixed value of 0.014. This value was derived from the median of a set of values for many (but not all) of the locations included in the IWAIR dispersion factor database.

$$K_{oc} = 10^{(\log K_{ow} - 0.32)} \qquad (6\text{-}11)$$

where

K_{ow} = octanol-water partition coefficient (L/kg).

Wastes can occur in the organic phase at concentrations below the soil saturation or solubility limit, as well as up to 1,000,000 mg/kg or mg/L (ppm). Regardless of whether the chemical is in the aqueous or organic phase, the concentration cannot exceed 1,000,000 mg/kg or mg/L (ppm) by definition. Therefore, IWAIR limits calculated allowable waste concentrations based on organic-phase emission rates to 1,000,000 ppm or lower.

As described in Sections 6.2.1 and 6.2.2, IWAIR calculates waste concentrations for both aqueous- and organic-phase emission rates. It then chooses between them using the following decision rules:

- If one of the two concentrations is physically impossible (greater than saturation or solubility limits for aqueous phase, or greater than 1,000,000 ppm for organic phase), it is discarded and the other is used.

- If both concentrations are impossible, then the allowable concentration is set to the saturation or solubility limit or 1,000,000 ppm, depending on which produces the higher risk. That risk is reported as the maximum achievable risk.

■   If both concentrations are physically possible, IWAIR selects the lower of the two. This is the lowest concentration that could produce the target risk. The underlying waste type (aqueous or organic) is reported. For most chemicals, this will be the concentration based on aqueous-phase emissions, as these are greater than the organic-phase emissions for the same concentration and, therefore, produce greater risk. Formaldehyde is a notable exception and has greater emissions (and therefore greater risk) from an organic-phase waste than an aqueous-phase waste.